LPSO formation mechanism based on the middle range ordering of small clusters

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The authors have performed the energetic assessments on the formation mechanism of Mg-LPSO structure. Quite recently, we've found that the interaction energy between the $L1_2$ cluster and a small cluster shows not a monotonous tendency but the slight minimum at the middle range of 4-5 layers. This slight middle range ordering invokes the long range stacking order observed in Mg-Zn-Y LPSO structures. We will survey the failures of the previously proposed mechanisms of LPSO formation, and report the detailed calculation models and results of middle range ordering.

The LPSO structure is formed by the synchronous interactions between the stacking fault and the $L1_2$ clusters. When we consider more specifically, two scenario are shortly proposed, where

1. stacking fault first then cluster, or
2. cluster first then stacking fault.

By the first principles calculations of the long period stacking structures indicated the slight tendency of the stabilization of 18R at the finite temperatures[1]. The energy difference between 18R and hcp, however, smaller than the 10meV/unit cell, which is easily hidden by the thermal fluctuation. On the other hand, Okuda *et al.* have recently observed the cluster first by the small angle scattering measurement in the formation of LPSO structure from the amorphous phase. We will show the energetic assessment of this cluster first scenario by the first principle calculation of VASP.

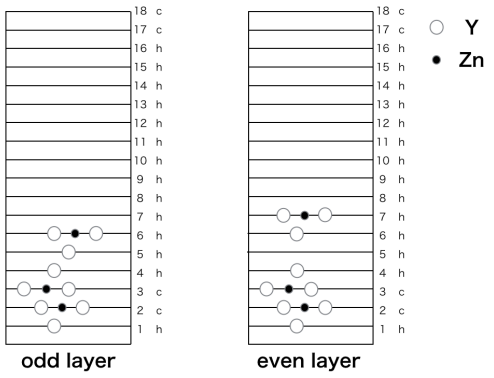

Figure 1: Schematic drawings of the side view of models.

Quite recently, Kiyohara *et al.* have reported that a horizontally split $L1_2$ cluster embedded in hcp lattice shows stable energy[2], whose size are close to those observed by Okuda *et al.*[3]. The energies of these smaller clusters embedded in the slab models with 18 and 24 stacking layers as shown in Fig.1 are obtained by VASP. The horizontally split cluster is embedded in each layer apart from a $L1_2$ cluster located at the stacking fault, as shown in Fig.1. The total energy change as shown in Fig.2 leads not a monotonous tendency but the slight minimum at the middle range of 4-5 layers apart from the stacking fault layer. This minimum induces the middle range ordering of the clusters.

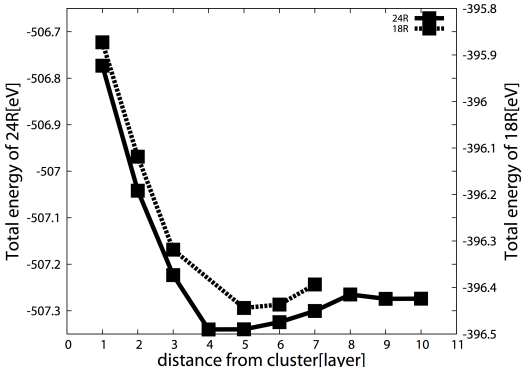

Figure 2: Interlayer distance dependency of interaction energy between $L1_2$ and smaller clusters.

References

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[3] H. Okuda, M. Yamasaki, Y. Kawamura, M. Tabuchi, H. Kimizuka: Scientific Reports **5** (2015), 14186.